10734306

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L2              0 S L1
L3                STRUCTURE UPLOADED
L4              2 S L3
L5              2 S L3
L6             30 S L3 SSS FULL

     FILE 'CAPLUS' ENTERED AT 17:18:44 ON 14 APR 2004

=> s l6
L7             8 L6

=> s l7 not thieno?
          7040 THIENO?
L8             8 L7 NOT THIENO?

=> d l1
L1 HAS NO ANSWERS
L1                STR
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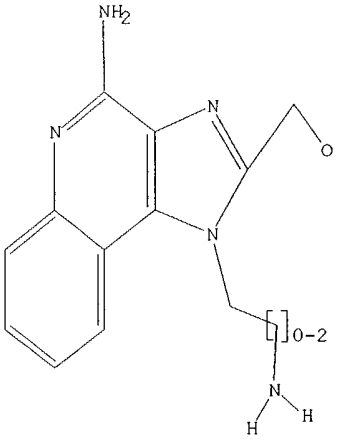

G1 C,O

Structure attributes must be viewed using STN Express query preparation.

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L3 HAS NO ANSWERS
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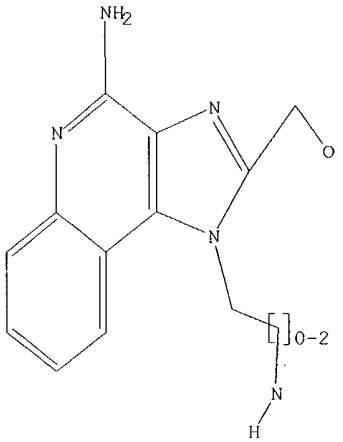


G1 C,O

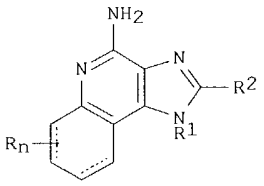
Structure attributes must be viewed using STN Express query preparation.

=> d 1-8 bib abs hitstr

L8 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:33981 CAPLUS
DN 140:94043
TI Preparation of imidazoquinolinesulfonamides as inducers of cytokine biosynthesis.
IN Griesgraber, George W.
PA 3M Innovative Properties Company, USA
SO U.S., 86 pp., Cont. of U.S. Ser. No. 27,273, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6677349	B1	20040113	US 2003-425054	20030428
PRAI US 2001-27273	B1	20011221		

OS MARPAT 140:94043
GI



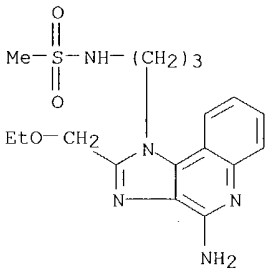
I

AB Title compds. [I; R1 = alkyl-NR3SO2XR4, alkenyl-NR3SO2XR4; X = bond, R5; R4 = (substituted) aryl, heteroaryl, heterocyclyl, alkyl, alkenyl; R2 = H, (substituted) alkyl, alkenyl, aryl, heteroaryl, alkyl-O-alkyl, alkyl-O-alkenyl; R3 = H, alkyl; R5 = H, alkyl; R4R5 = atoms to form a 3-7 membered (substituted) heterocyclyl; n = 0-4; R = alkyl, alkoxy, halo, CF3], were prepared Thus, a stirred solution of 4-chloro-3-nitroquinoline in CH2Cl2 was treated with Et3N and 1,2-diamino-2-methylpropane to give 2-methyl-N1-(3-nitroquinolin-4-yl)propane-1,2-diamine. A solution of the latter in THF was cooled to 0° and treated with a 1 N NaOH solution of di-tert-Bu dicarbonate under rapid stirring followed by warming to ambient temperature and stirring overnight; addnl. di-tert-Bu dicarbonate was added and stirring was continued for 3 d. to give tert-Bu 1,1-dimethyl-2-[(3-nitroquinolin-4-yl)amino]ethylcarbamate. This in PhMe was treated with Pt/C and shaken under H2 for 6 h to give tert-Bu 2-(3-aminoquinolin-4-yl)-1,1-dimethylethylcarbamate. The aminoquinoline in CH2Cl2 was cooled to 0° and treated with Et3N and ethoxyacetyl chloride to give a syrup which was refluxed overnight with Et3N in EtOH to give tert-Bu 2-[2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethylcarbamate. The imidazoquinoline in CH2Cl2 was treated with 3-chloroperoxybenzoic acid and stirred 2 h to give tert-Bu 2-[2-(ethoxymethyl)-5-oxido-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethylcarbamate. The latter in 1,2-dichloroethane was heated to 70° and treated with concentrated NH4OH; p-toluenesulfonyl chloride was added and the reaction mixture was heated in a sealed tube for 2 h to give tert-Bu 2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethylcarbamate . This was refluxed in EtOH containing HCl for 2 h to give 1-(2-amino-2-methylpropyl)-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-4-amine. 1-(2-Amino-2-methylpropyl)-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-4-amine in CH2Cl2 at 0° was treated with Et3N and MeSO2Cl and the reaction was allowed to warm to ambient temperature overnight to give N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethyl]methanesulfonamide (claimed compound). I induced interferon in an in vitro human blood cell system at lowest effective concns. of 0.0001-10 μM.

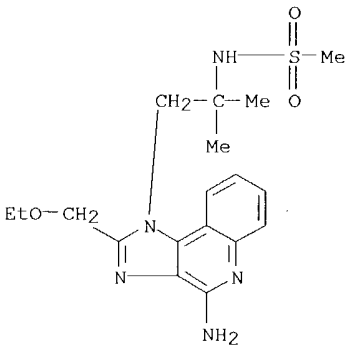
IT **642473-53-8P 642473-62-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of imidazoquinolinesulfonamides as inducers of cytokine biosynthesis)

RN 642473-53-8 CAPLUS
CN Methanesulfonamide, N-[3-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]propyl]- (9CI) (CA INDEX NAME)

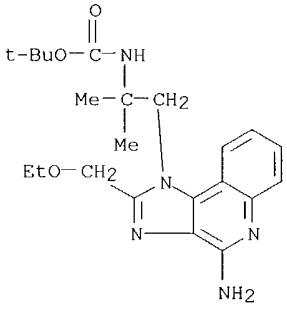


RN 642473-62-9 CAPLUS
CN Methanesulfonamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethyl]- (9CI) (CA INDEX NAME)

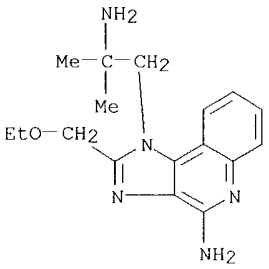


IT **642473-94-7P 642473-95-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of imidazoquinolinesulfonamides as inducers of cytokine biosynthesis)

RN 642473-94-7 CAPLUS
CN Carbamic acid, [2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 642473-95-8 CAPLUS
CN 1H-Imidazo[4,5-c]quinoline-1-ethanamine, 4-amino-2-(ethoxymethyl)-α,α-dimethyl- (9CI) (CA INDEX NAME)

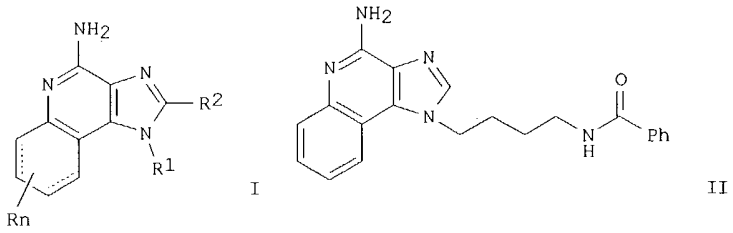


RE.CNT 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:590833 CAPLUS
DN 139:149629
TI Preparation of amidoimidazo[4,5-c]quinolines as immune response modifiers
IN Coleman, Patrick L.; Crooks, Stephen L.; Griesgraber, George W.; Lindstrom, Kyle J.; Merrill, Bryon A.; Rice, Michael J.
PA USA
SO U.S. Pat. Appl. Publ., 85 pp., Cont.-in-part of U.S. 6,451,810.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003144283	A1	20030731	US 2001-27218	20011221
	US 6451810	B1	20020917	US 2000-589580	20000607
	ZA 2001009854	A	20030228	ZA 2001-9854	20011129
	ZA 2001009857	A	20030228	ZA 2001-9857	20011129
	ZA 2001009861	A	20030228	ZA 2001-9861	20011129
	US 2004029877	A1	20040212	US 2001-27272	20011221
PRAI	US 1999-138365P	P	19990610		
	US 2000-589580	A2	20000607		
	US 2000-589216	A1	20000607		
	US 2001-166321	A1	20010615		

OS MARPAT 139:149629
GI



AB Title compds. I [wherein R1 = alkyl-NR3COR4; R3 = independently H, alkyl or (un)substituted alkyl(hetero)aryl; R4 = alkyl or (un)substituted (hetero)aryl; R2 = H, alkenyl, (un)substituted alkyl or (hetero)aryl, etc.; R = independently alkyl, alkoxy, halo, CF3; n = 0-4; and their pharmaceutically acceptable salts] were prepared as immune response modifiers. For example, II was prepared by acylation of 1-(4-aminobutyl)-1H-imidazo[4,5-c]quinolin-4-amine with benzoyl chloride in pyridine. II induced interferon α and TNFα at concns. of 0.37 μM and 10 μM, resp., in human cells. Thus, I and their pharmaceutical compns. are useful for the treatment of a variety of conditions including viral diseases and neoplastic diseases (no data).

IT **313347-68-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(immune response modifier; preparation of (amido)imidazo[4,5-c]quinolines as immune response modifiers)

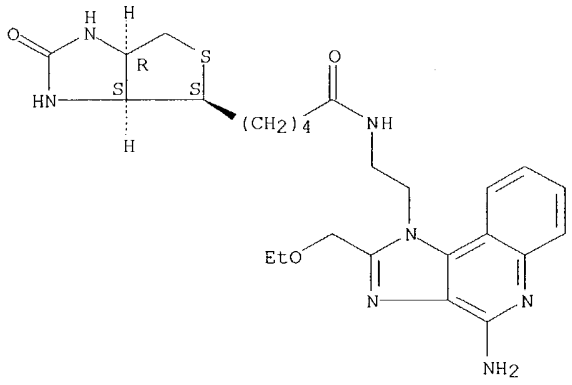
RN 313347-68-1 CAPLUS

CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]hexahydro-2-oxo-, (3aS,4S,6aR)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

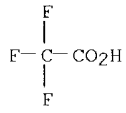
CRN 313347-67-0
CMF C25 H33 N7 O3 S

Absolute stereochemistry.



CM 2

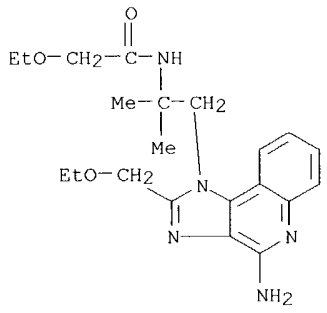
CRN 76-05-1
CMF C2 H F3 O2



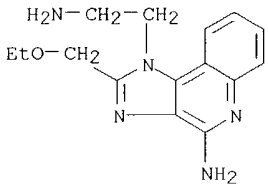
IT **570411-23-3P,** N-[2-[4-Amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethyl]-2-ethoxyacetamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(immune response modifiers; preparation of (amido)imidazo[4,5-c]quinolines as immune response modifiers)

RN 570411-23-3 CAPLUS

CN Acetamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethyl]-2-ethoxy- (9CI) (CA INDEX NAME)



IT **313350-40-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (amido)imidazo[4,5-c]quinolines as immune response modifiers)
RN 313350-40-2 CAPLUS
CN 1H-Imidazo[4,5-c]quinoline-1-ethanamine, 4-amino-2-(ethoxymethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

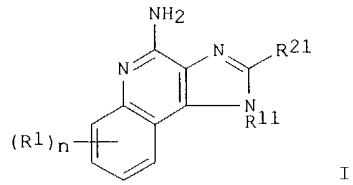


● HCl

L8 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:434369 CAPLUS
DN 139:26620
TI Topical pharmaceuticals comprising an immune response modifier
IN Skwierczynski, Raymond D.; Busch, Terri F.; Gust-Heiting, Amy L.; Fretland, Mary T.; Scholz, Matthew T.
PA 3M Innovative Properties Company, USA
SO PCT Int. Appl., 123 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003045391	A1	20030605	WO 2002-US38190	20021127
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003199538	A1	20031023	US 2002-306019	20021127
PRAI US 2001-340605P	P	20011129		
US 2002-378452P	P	20020506		

OS MARPAT 139:26620
GI



I

AB Pharmaceutical formulations comprise an immune response modifier (IRM) chosen from imidazoquinoline amines, imidazotetrahydroquinoline amines, imidazopyridine amines, and other heterocyclic fused ring derivs.; a fatty acid; and a hydrophobic, aprotic component miscible with the fatty acid are useful for the treatment of dermal associated conditions. Topical

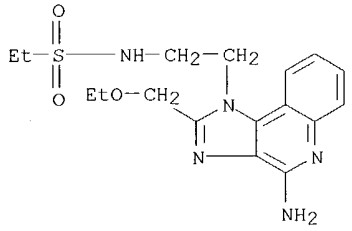
formulations containing, e.g., I are provided. In one embodiment, the topical formulations are advantageous for treatment of actinic keratosis, postsurgical scars, basal cell carcinoma, atopic dermatitis, and warts.

IT **534568-83-7 534568-84-8 534568-86-0 534568-89-3**

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(topical pharmaceuticals comprising an immune response modifier)

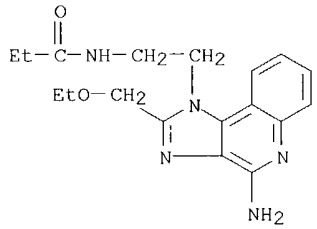
RN 534568-83-7 CAPLUS

CN Ethanesulfonamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]- (9CI) (CA INDEX NAME)



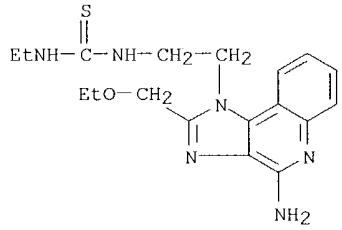
RN 534568-84-8 CAPLUS

CN Propanamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]- (9CI) (CA INDEX NAME)



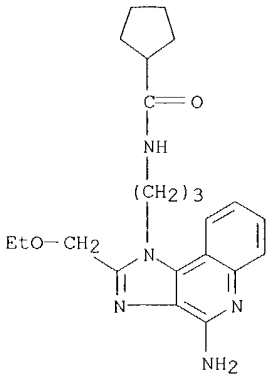
RN 534568-86-0 CAPLUS

CN Thiourea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-ethyl- (9CI) (CA INDEX NAME)



RN 534568-89-3 CAPLUS

CN Cyclopentanecarboxamide, N-[3-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]propyl]- (9CI) (CA INDEX NAME)

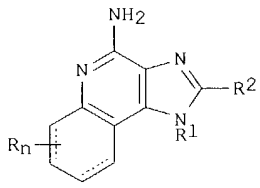


RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:429098 CAPLUS
DN 139:6873
TI Preparation of imidazoquinolinamines as immune response modifiers.
IN Crooks, Stephen L.; Griesgraber, George W.; Lindstrom, Kyle J.; Merrill, Bryon A.; Rice, Michael J.
PA 3M Innovative Properties Company, USA
SO U.S., 66 pp., Cont.-in-part of U.S. 6,541,485.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6573273	B1	20030603	US 2001-28255	20011221
	US 6541485	B1	20030401	US 2000-589236	20000607
	ZA 2001009854	A	20030228	ZA 2001-9854	20011129
	ZA 2001009857	A	20030228	ZA 2001-9857	20011129
	ZA 2001009861	A	20030228	ZA 2001-9861	20011129
	US 2004029877	A1	20040212	US 2001-27272	20011221
	US 2004014754	A1	20040122	US 2003-352604	20030128
	US 2004019048	A1	20040129	US 2003-370800	20030220
PRAI	US 1999-138365P	P	19990610		
	US 2000-589236	A2	20000607		
	US 2000-589216	A1	20000607		
	US 2001-166321	A1	20010615		
	US 2001-28255	A1	20011221		

OS MARPAT 139:6873
GI



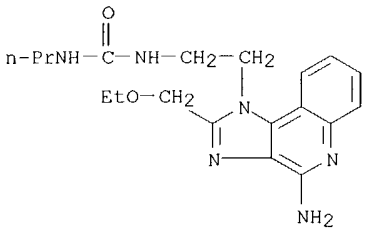
I

AB Title compds. [I; R1 = ANR3CYNR5XR4; A = alkylene, alkenylene; Y = O, S; X = bond, CO, SO2; R3 = H, alkyl; R4 = (substituted) aryl, heteroaryl, alkyl, etc.; R5 = H, alkyl; R4R5 = atoms to form 3-7 membered (un)substituted heterocyclic ring; R2 = H, alkyl,aryl, etc.; R = alkyl, alkoxy, halo, CF3; n = 0-4], were prepared Thus, reaction of 4-morpholinecarbonyl chloride with 1-(4-aminobutyl)-1H-imidazo[4,5-c]quinolin-4-amine in pyridine afforded N4-[4-[4-amino-1H-imidazo[4,5-c]quinolin-1-yl]butyl]-4-morpholinecarboxamide which induced interferon-α biosynthesis in human cells at a lowest concentration of 3.33

μM.

IT **313383-61-8P 313383-62-9P 313383-63-0P**
313383-64-1P 313383-65-2P 313383-66-3P
313385-13-6P 313385-28-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of imidazoquinolinamines as immune response modifiers)

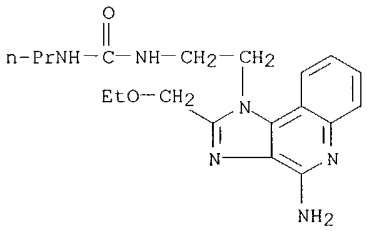
RN 313383-61-8 CAPLUS
CN Urea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-propyl- (9CI) (CA INDEX NAME)



RN 313383-62-9 CAPLUS
CN Urea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-propyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

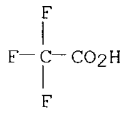
CM 1

CRN 313383-61-8
CMF C19 H26 N6 O2

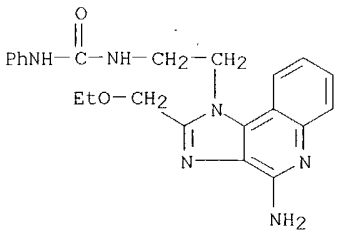


CM 2

CRN 76-05-1
CMF C2 H F3 O2



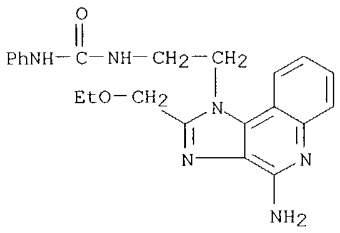
RN 313383-63-0 CAPLUS
CN Urea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-phenyl- (9CI) (CA INDEX NAME)



RN 313383-64-1 CAPLUS
CN Urea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-phenyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

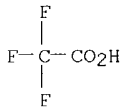
CM 1

CRN 313383-63-0
CMF C22 H24 N6 O2

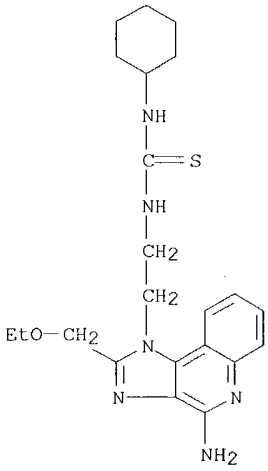


CM 2

CRN 76-05-1
CMF C2 H F3 O2



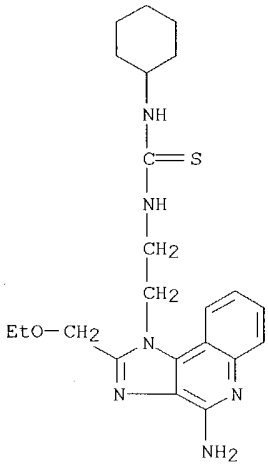
RN 313383-65-2 CAPLUS
CN Thiourea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-cyclohexyl- (9CI) (CA INDEX NAME)



RN 313383-66-3 CAPLUS
CN Thiourea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-cyclohexyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

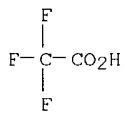
CM 1

CRN 313383-65-2
CMF C22 H30 N6 O S

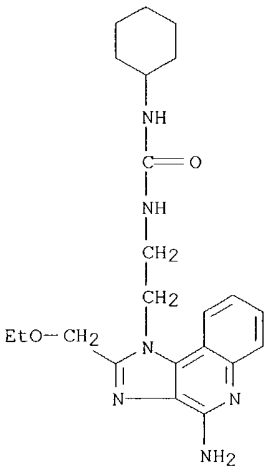


CM 2

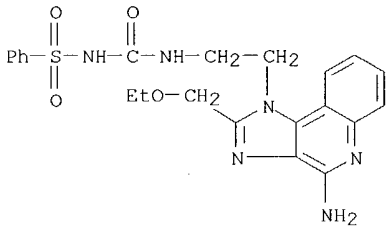
CRN 76-05-1
CMF C2 H F3 O2



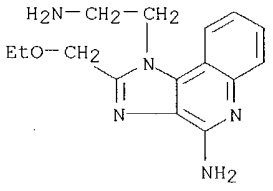
RN 313385-13-6 CAPLUS
CN Urea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-cyclohexyl- (9CI) (CA INDEX NAME)



RN 313385-28-3 CAPLUS
CN Benzenesulfonamide, N-[[[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]amino]carbonyl]- (9CI) (CA INDEX NAME)



IT **313350-40-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of imidazoquinolinamines as immune response modifiers)
RN 313350-40-2 CAPLUS
CN 1H-Imidazo[4,5-c]quinoline-1-ethanamine, 4-amino-2-(ethoxymethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

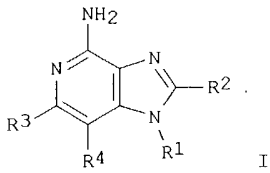
L8 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:360094 CAPLUS
DN 134:366874
TI Preparation of dye-labeled imidazoquinolines and analogs as immunomodulators
IN Wei, Ai-Ping; Tomai, Mark A.; Rice, Michael J.

10734306

PA 3M Innovative Properties Company, USA
SO PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001034709	A1	20010517	WO 2000-US30366	20001103
	W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6376669	B1	20020423	US 2000-705072	20001102
	EP 1228147	A1	20020807	EP 2000-980282	20001103
	EP 1228147	B1	20040204		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004500347	T2	20040108	JP 2001-537411	20001103
	AT 258963	E	20040215	AT 2000-980282	20001103
	US 2002120141	A1	20020829	US 2002-78645	20020219
	US 6630588	B2	20031007		
	NO 2002001974	A	20020628	NO 2002-1974	20020425
PRAI	US 1999-163724P	P	19991105		
	US 2000-705072	A	20001102		
	WO 2000-US30366	W	20001103		

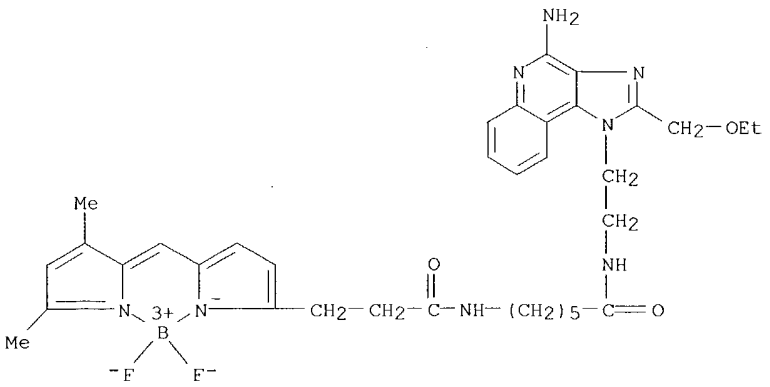
OS MARPAT 134:366874
GI



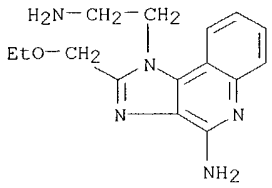
I

AB Title compds. [I; R1 = ZR; R = dye residue; R2 = H, (un)substituted alkyl, (hetero)aryl(alkyl), etc.; R3,R4 = H, halo, alkyl, alkoxy, etc.; R3R4 = atoms to complete a ring; Z = spacer group], useful, inter alia, for determining the binding and/or receptor sites of the mols., were prepared Thus, 3-nitro-4-quinolinol was aminated by H2N(CH2)4CHCO2CMe3 and the reduced product cyclocondensed with MeOCH2CH2COCl to give, in 3 addnl. steps, I [R1 = (CH2)4NHR, R2 = CH2CH2OMe, R3R4 = CH:CHCH:CH](II; R = H) which was amidated by fluorescein 5-isothiocyanate to give II (R = CSNHZ1R5, R5 = 6-hydroxy-3-oxo-3H-xanthen-9-yl, Z1 = 3-carboxy-1,4-phenylene). Data for biol. activity of 1 prepared I were given.

IT **340128-24-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dye-labeled imidazoquinolines and analogs as immunomodulators)
RN 340128-24-7 CAPLUS
CN Boron, [N-[6-[[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]amino]-6-oxohexyl]-5-[(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrole-2-propanamidato-κN1]difluoro-, (T-4)-(9CI) (CA INDEX NAME)



IT **339545-53-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dye-labeled imidazoquinolines and analogs as immunomodulators)
RN 339545-53-8 CAPLUS
CN 1H-Imidazo[4,5-c]quinoline-1-ethanamine, 4-amino-2-(ethoxymethyl)-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

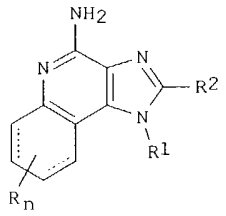
L8 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:900462 CAPLUS
DN 134:56667
TI Preparation of sulfonamide and sulfamide substituted imidazoquinolines as immune response modifiers
IN Crooks, Stephen L.; Lindstrom, Kyle J.; Merrill, Bryon A.; Rice, Michael J.
PA 3M Innovative Properties Company, USA
SO PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000076519	A1	20001221	WO 2000-US15722	20000608
	W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6331539	B1	20011218	US 2000-589216	20000607
	BR 2000011433	A	20020305	BR 2000-11433	20000608

	EP 1198233	A1	20020424	EP 2000-938211	20000608
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2003501474	T2	20030114	JP 2001-502852	20000608
	EE 200100669	A	20030217	EE 2001-669	20000608
	NZ 515967	A	20031031	NZ 2000-515967	20000608
	US 2003130299	A1	20030710	US 2001-166321	20010615
	NO 2001005502	A	20020207	NO 2001-5502	20011109
	ZA 2001009854	A	20030228	ZA 2001-9854	20011129
	ZA 2001009857	A	20030228	ZA 2001-9857	20011129
	ZA 2001009861	A	20030228	ZA 2001-9861	20011129
	HR 2001000890	A1	20030831	HR 2001-890	20011129
	US 2004029877	A1	20040212	US 2001-27272	20011221
PRAI	US 1999-138365P	P	19990610		
	US 2000-589216	A	20000607		
	WO 2000-US15722	W	20000608		
	US 2001-166321	A1	20010615		

OS MARPAT 134:56667

GI



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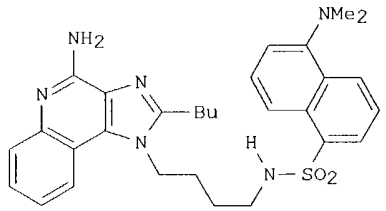


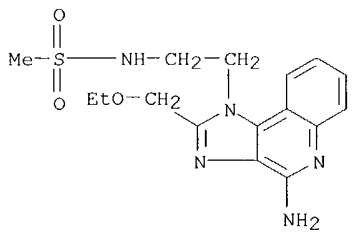
II

AB The title compds. [I; R1 = alkylNR3SO2XR4, alkenylNR3SO2XR4 (wherein X = a bond, NR5; R3 = H, alkyl; R4 = (un)substituted aryl, heteroaryl, alkyl, etc.; R5 = H, alkyl; R4 and R5 can combine to form 3-7 membered (un)substituted heterocyclic ring); R2 = H, alkyl, aryl, etc.; R = alkyl, alkoxy, halo, CF3; n = 0-4], useful as immune response modifiers, were prepared Thus, reacting 5-dimethylamino-1-naphthalenesulfonyl chloride with 1-(4-aminobutyl)-2-butyl-1H-imidazo[4,5-c]quinolin-4-amine in the presence of N,N-diisopropylethylamine in CH2Cl2 afforded the naphthalenesulfonamide II which induced interferon α and TNFα biosynthesis in human cells at 0.12 μM and 3.33 μM, resp. The compds. I can induce the biosynthesis of various cytokines such as interferon α and TNFα (data given), and are useful in the treatment of a variety of conditions including viral diseases and neoplastic diseases.

IT **313357-78-7P 313357-79-8P 313357-80-1P**
313357-81-2P 313357-82-3P 313357-83-4P
313360-03-1P 313360-04-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of sulfonamide and sulfamide substituted imidazoquinolines as immune response modifiers)

RN 313357-78-7 CAPLUS

CN Methanesulfonamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]- (9CI) (CA INDEX NAME)

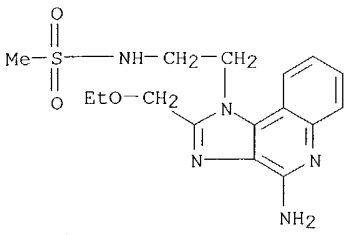


RN 313357-79-8 CAPLUS

CN Methanesulfonamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

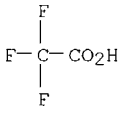
CM 1

CRN 313357-78-7
CMF C16 H21 N5 O3 S

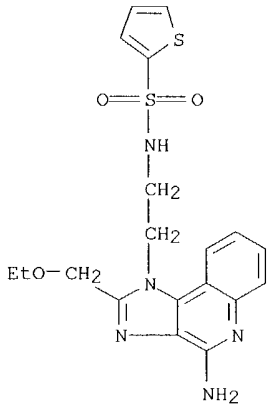


CM 2

CRN 76-05-1
CMF C2 H F3 O2



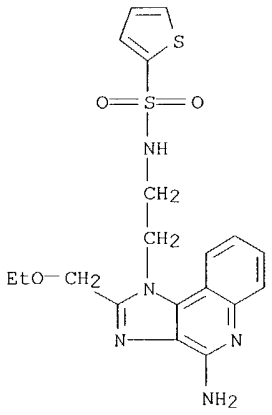
RN 313357-80-1 CAPLUS
CN 2-Thiophenesulfonamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]- (9CI) (CA INDEX NAME)



RN 313357-81-2 CAPLUS
CN 2-Thiophenesulfonamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

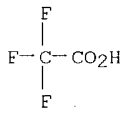
CM 1

CRN 313357-80-1
CMF C19 H21 N5 O3 S2

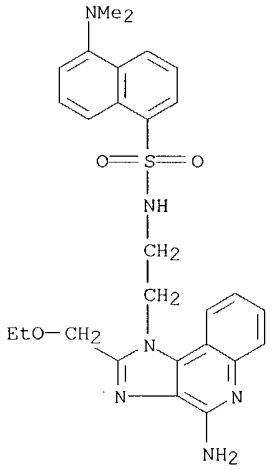


CM 2

CRN 76-05-1
CMF C2 H F3 O2



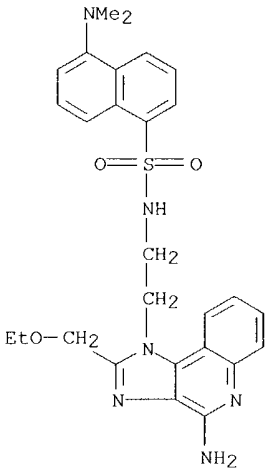
RN 313357-82-3 CAPLUS
CN 1-Naphthalenesulfonamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-5-(dimethylamino)- (9CI) (CA INDEX NAME)



RN 313357-83-4 CAPLUS
CN 1-Naphthalenesulfonamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-5-(dimethylamino)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

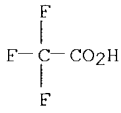
CM 1

CRN 313357-82-3
CMF C27 H30 N6 O3 S

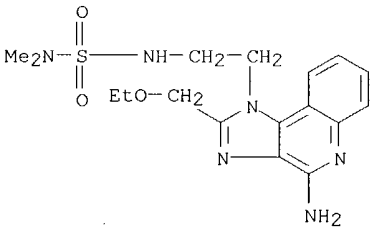


CM 2

CRN 76-05-1
CMF C2 H F3 O2



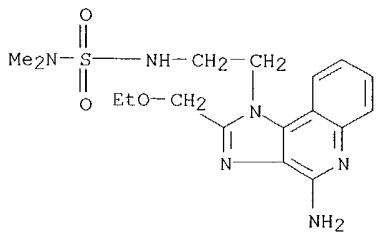
RN 313360-03-1 CAPLUS
CN Sulfamide, N'-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 313360-04-2 CAPLUS
CN Sulfamide, N'-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N,N-dimethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

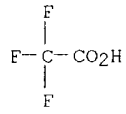
CM 1

CRN 313360-03-1
CMF C17 H24 N6 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:900461 CAPLUS
DN 134:56666
TI Preparation of urea substituted imidazoquinolines as immune response modifiers
IN Crooks, Stephen L.; Merrill, Bryon A.; Rice, Michael J.
PA 3M Innovative Properties Company, USA
SO PCT Int. Appl., 106 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000076518	A1	20001221	WO 2000-US15656	20000608
	W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6541485	B1	20030401	US 2000-589236	20000607
	EP 1198232	A1	20020424	EP 2000-938205	20000608
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	JP 2003501473	T2	20030114	JP 2001-502851	20000608
	EE 200100668	A	20030217	EE 2001-668	20000608
	AU 766565	B2	20031016	AU 2000-53281	20000608
	NZ 515968	A	20031031	NZ 2000-515968	20000608
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	ZA 2001009857	A	20030228	ZA 2001-9857	20011129
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	HR 2001000889	A1	20030831	HR 2001-889	20011129
	US 2004029877	A1	20040212	US 2001-27272	20011221
	US 2004014754	A1	20040122	US 2003-352604	20030128
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	US 2000-589236	A	20000607		
	US 2000-589216	A1	20000607		
	WO 2000-US15656	W	20000608		
	US 2001-166321	A1	20010615		

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OS MARPAT 134:56666
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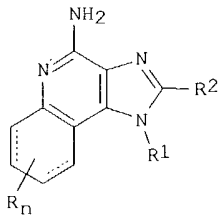

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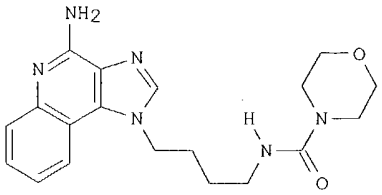
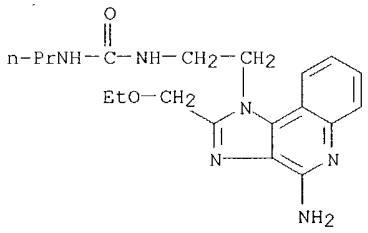


II

AB The title compds. [I; R1 = alkylNR3CYNR5XR4, alkenylNR3CYNR5XR4 (wherein Y = O, S; X = a bond, CO, SO2; R3 = H, alkyl; R4 = (un)substituted aryl, heteroaryl, alkyl, etc.; R5 = H, alkyl; R4 and R5 can combine to form 3-7 membered (un)substituted heterocyclic ring); R2 = H, alkyl,aryl, etc.; R = alkyl, alkoxy, halo, CF3; n = 0-4], useful as immune response modifiers, were prepared Thus, reacting 4-morpholinecarbonyl chloride with 1-(4-aminobutyl)-1H-imidazo[4,5-c]quinolin-4-amine in pyridine afforded II which induced interferon α biosynthesis in human cells at 3.33 μM. The compds. I can induce the biosynthesis of various cytokines such as interferon α and TNFα (data given), and are useful in the treatment of a variety of conditions including viral diseases and neoplastic diseases.

IT **313383-61-8P 313383-62-9P 313383-63-0P**
313383-64-1P 313383-65-2P 313383-66-3P
313385-13-6P 313385-28-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of urea substituted imidazoquinolines as immune response modifiers)

RN 313383-61-8 CAPLUS
CN Urea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-propyl- (9CI) (CA INDEX NAME)



RN 313383-62-9 CAPLUS
CN Urea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-propyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 313383-61-8
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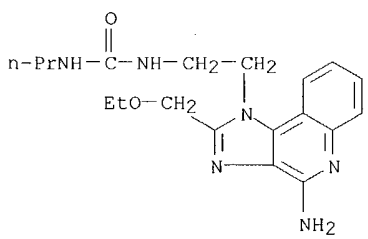

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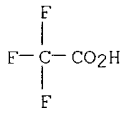
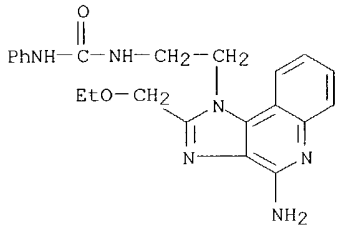


RN 313383-63-0 CAPLUS
CN Urea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-phenyl- (9CI) (CA INDEX NAME)



RN 313383-64-1 CAPLUS
CN Urea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-phenyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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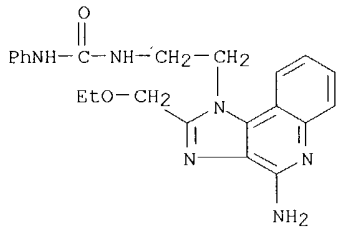

CM 2

CRN 76-05-1
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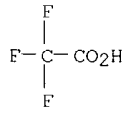
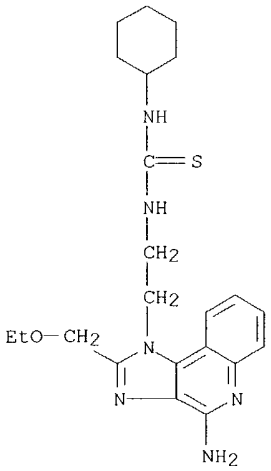


RN 313383-65-2 CAPLUS
CN Thiourea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-cyclohexyl- (9CI) (CA INDEX NAME)



RN 313383-66-3 CAPLUS
CN Thiourea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-N'-cyclohexyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

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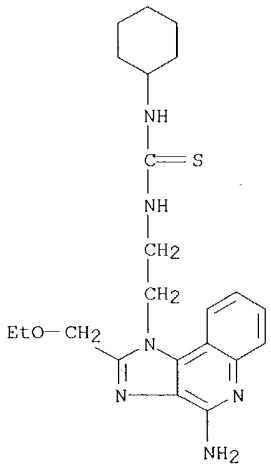
CMF C22 H30 N6 O S



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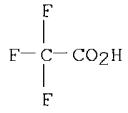
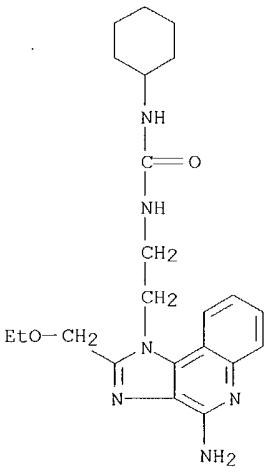
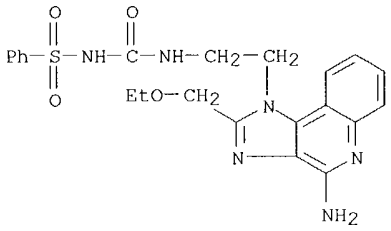


RN 313385-13-6 CAPLUS
CN Urea, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]-

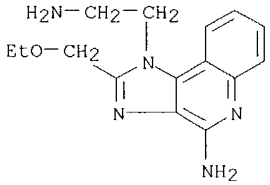
N'-cyclohexyl- (9CI) (CA INDEX NAME)



RN 313385-28-3 CAPLUS
CN Benzenesulfonamide, N-[[[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]amino]carbonyl]- (9CI) (CA INDEX NAME)



IT **313350-40-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of urea substituted imidazoquinolines as immune response modifiers)
RN 313350-40-2 CAPLUS
CN 1H-Imidazo[4,5-c]quinoline-1-ethanamine, 4-amino-2-(ethoxymethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:900448 CAPLUS
DN 134:56665
TI Preparation of amide substituted imidazoquinolines as immune response

modifiers
IN Coleman, Patrick L.; Crooks, Stephen L.; Lindstrom, Kyle J.; Merrill, Bryon A.; Rice, Michael J.
PA 3M Innovative Properties Company, USA
SO PCT Int. Appl., 170 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000076505	A1	20001221	WO 2000-US15702	20000608
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	US 6451810	B1	20020917	US 2000-589580	20000607
	EP 1187613	A1	20020320	EP 2000-950215	20000608
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	EE 200100670	A	20030217	EE 2001-670	20000608
	NO 2001005503	A	20020208	NO 2001-5503	20011109
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	ZA 2001009857	A	20030228	ZA 2001-9857	20011129
	ZA 2001009861	A	20030228	ZA 2001-9861	20011129
	HR 2001000888	A1	20030831	HR 2001-888	20011129
	US 2004029877	A1	20040212	US 2001-27272	20011221
PRAI	US 1999-138365P	P	19990610		
	US 2000-589580	A	20000607		
	US 2000-589216	A1	20000607		
	WO 2000-US15702	W	20000608		
	US 2001-166321	A1	20010615		

OS MARPAT 134:56665
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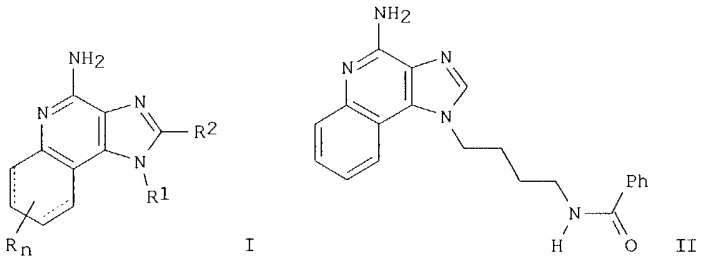
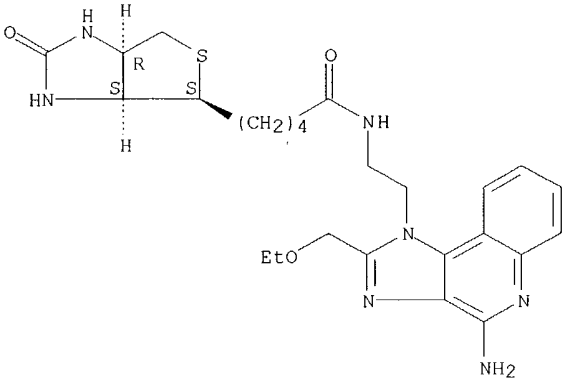


AB The title compds. [I; R1 = alkylNR3COR4, alkenylNR3COR4 (wherein R4 = (un)substituted aryl, heteroaryl, alkyl, etc.); R2 = H, alkyl, alkenyl, etc.; R = alkyl, alkoxy, halo, CF3; n = 0-4] and their pharmaceutically acceptable salts, useful as immune response modifiers, were prepared Thus, reacting 1-(4-aminobutyl)-1H-imidazo[4,5-c]quinolin-4-amine with benzoyl chloride in pyridine afforded the benzamide II which showed the lowest concentration of 0.37 μM to induce interferon in human cells. The compds. I can induce the biosynthesis of various cytokines (data given for interferon α and TNFα) and are useful in the treatment of a variety of conditions including viral diseases and neoplastic diseases.
IT **313347-67-0P 313347-68-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amide substituted imidazoquinolines as immune response modifiers)
RN 313347-67-0 CAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-

imidazo[4,5-c]quinolin-1-yl]ethyl]hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 313347-68-1 CAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]ethyl]hexahydro-2-oxo-, (3aS,4S,6aR)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

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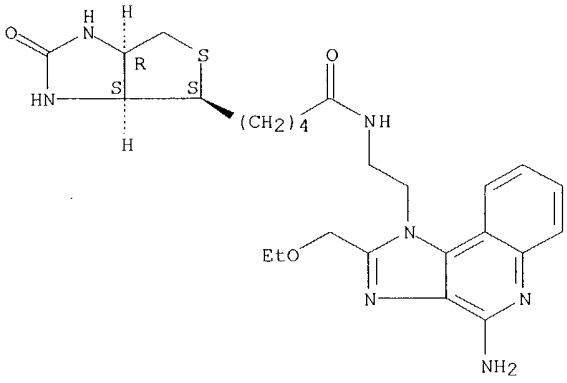
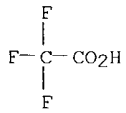
Absolute stereochemistry.



CM 2

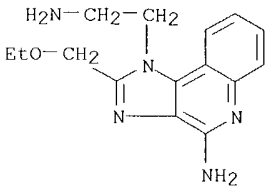
CRN 76-05-1
CMF C2 H F3 O2



IT **313350-40-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amide substituted imidazoquinolines as immune response modifiers)

10734306

RN 313350-40-2 CAPLUS
CN 1H-Imidazo[4,5-c]quinoline-1-ethanamine, 4-amino-2-(ethoxymethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



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RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10734306

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L2             1 S L1
L3            15 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 15:32:38 ON 14 APR 2004
L4             3 S L3

     FILE 'REGISTRY' ENTERED AT 15:38:48 ON 14 APR 2004
L5               STRUCTURE UPLOADED
L6             4 S L5
L7            66 S L5 SSS FULL
L8            51 S L7 NOT L3

     FILE 'CAPLUS' ENTERED AT 15:40:29 ON 14 APR 2004
L9             4 S L8
                 SELECT L9 1 RN

     FILE 'REGISTRY' ENTERED AT 16:28:16 ON 14 APR 2004
L10          337 S E1-E337
L11           12 S L10 AND ETHOXYMETHYL

=> s l11 and C17 H23 N5 O/mf
          188 C17 H23 N5 O/MF
L12           1 L11 AND C17 H23 N5 O/MF

=> d scan

L12  1 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN   1H-Imidazo[4,5-c]quinoline-1-ethanamine, 4-amino-2-(ethoxymethyl)-
     α,α-dimethyl- (9CI)
MF   C17 H23 N5 O
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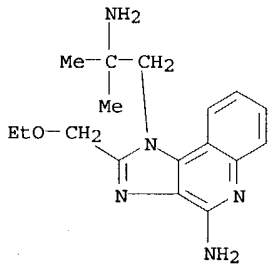


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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**


ALL ANSWERS HAVE BEEN SCANNED


=> d all

L12  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   642473-95-8  REGISTRY
ED   Entered STN:  28 Jan 2004
CN   1H-Imidazo[4,5-c]quinoline-1-ethanamine, 4-amino-2-(ethoxymethyl)-
     α,α-dimethyl- (9CI)     (CA INDEX NAME)
MF   C17 H23 N5 O
SR   CA
LC   STN Files:   CA, CAPLUS, USPATFULL

Ring System Data
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Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
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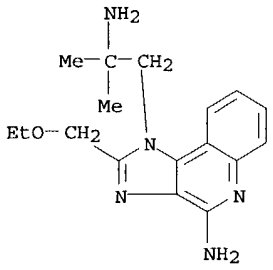
10734306



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
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Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	9.23	pH 10	(1) ACD
Boiling Point (BP)	538.8+/-50.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	81.60+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	279.6+/-54.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	4		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	2.54	pH 8	(1) ACD
Koc (KOC)	160	pH 10	(1) ACD
logD (LOGD)	-3.29	pH 1	(1) ACD
logD (LOGD)	-3.29	pH 4	(1) ACD
logD (LOGD)	-1.98	pH 7	(1) ACD
logD (LOGD)	-0.19	pH 8	(1) ACD
logD (LOGD)	1.60	pH 10	(1) ACD
logP (LOGP)	1.707+/-1.125		(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	313.40		(1) ACD
pKa (PKA)	9.15+/-0.50	Most Basic	(1) ACD
Vapor Pressure (VP)	1.12E-11 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

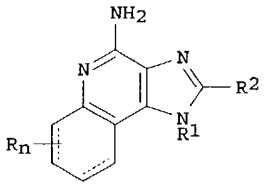
AN 140:94043 CA
TI Preparation of imidazoquinolinesulfonamides as inducers of cytokine biosynthesis.
IN Griesgraber, George W.
PA 3M Innovative Properties Company, USA
SO U.S., 86 pp., Cont. of U.S. Ser. No. 27,273, abandoned.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-4745
ICS A61K031-541; C07D471-04; C07D417-14; A61P037-02

10734306

NCL 514293000
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6677349	B1	20040113	US 2003-425054	20030428
PRAI	US 2001-27273	20011221			

GI



I

AB Title compds. [I; R1 = alkyl-NR3SO2XR4, alkenyl-NR3SO2XR4; X = bond, R5; R4 = (substituted) aryl, heteroaryl, heterocyclyl, alkyl, alkenyl; R2 = H, (substituted) alkyl, alkenyl, aryl, heteroaryl, alkyl-O-alkyl, alkyl-O-alkenyl; R3 = H, alkyl; R5 = H, alkyl; R4R5 = atoms to form a 3-7 membered (substituted) heterocyclyl; n = 0-4; R = alkyl, alkoxy, halo, CF3], were prepared Thus, a stirred solution of 4-chloro-3-nitroquinoline in CH2Cl2 was treated with Et3N and 1,2-diamino-2-methylpropane to give 2-methyl-N1-(3-nitroquinolin-4-yl)propane-1,2-diamine. A solution of the latter in THF was cooled to 0° and treated with a 1 N NaOH solution of di-tert-Bu dicarbonate under rapid stirring followed by warming to ambient temperature and stirring overnight; addnl. di-tert-Bu dicarbonate was added and stirring was continued for 3 d. to give tert-Bu 1,1-dimethyl-2-[(3-nitroquinolin-4-yl)amino]ethylcarbamate. This in PhMe was treated with Pt/C and shaken under H2 for 6 h to give tert-Bu 2-(3-aminoquinolin-4-yl)-1,1-dimethylethylcarbamate. The aminoquinoline in CH2Cl2 was cooled to 0° and treated with Et3N and ethoxyacetyl chloride to give a syrup which was refluxed overnight with Et3N in EtOH to give tert-Bu 2-[2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethylcarbamate. The imidazoquinoline in CH2Cl2 was treated with 3-chloroperoxybenzoic acid and stirred 2 h to give tert-Bu 2-[2-(ethoxymethyl)-5-oxido-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethylcarbamate. The latter in 1,2-dichloroethane was heated to 70° and treated with concentrated NH4OH; p-toluenesulfonyl chloride was added and the reaction mixture was heated in a sealed tube for 2 h to give tert-Bu 2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethylcarbamate . This was refluxed in EtOH containing HCl for 2 h to give 1-(2-amino-2-methylpropyl)-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-4-amine. 1-(2-Amino-2-methylpropyl)-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-4-amine in CH2Cl2 at 0° was treated with Et3N and MeSO2Cl and the reaction was allowed to warm to ambient temperature overnight to give N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethyl]methanesulfonamide (claimed compound). I induced interferon in an in vitro human blood cell system at lowest effective concns. of 0.0001-10 μM.

ST imidazoquinolinesulfonamide prepn cytokine biosynthesis inhibitor; interferon tumor necrosis factor induction imidazoquinolinesulfonamide prepn

IT Cytokines
Interferons
Tumor necrosis factors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inducers; preparation of imidazoquinolinesulfonamides as inducers of cytokine biosynthesis)

IT Drug delivery systems
Human
(preparation of imidazoquinolinesulfonamides as inducers of cytokine biosynthesis)

IT 313355-83-8P 313355-85-0P 313355-87-2P 313355-89-4P 313355-90-7P
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(preparation of imidazoquinolinesulfonamides as inducers of cytokine biosynthesis)

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642473-63-0P 642473-65-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of imidazoquinolinesulfonamides as inducers of cytokine biosynthesis)

IT 642473-24-3 642473-26-5
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(preparation of imidazoquinolinesulfonamides as inducers of cytokine biosynthesis)

IT 98-09-9, Benzenesulfonyl chloride 98-74-8, 4-Nitrobenzenesulfonyl chloride 121-51-7, 3-Nitrobenzenesulfonyl chloride 124-63-0, Methanesulfonyl chloride 349-88-2, 4-Fluorobenzenesulfonyl chloride 358-23-6, Trifluoromethanesulfonic anhydride 594-44-5, Ethanesulfonyl chloride 605-65-2, 5-Dimethylamino-1-naphthalenesulfonyl chloride 811-93-8, 1,2-Diamino-2-methylpropane 1633-82-5, 3-Chloropropylsulfonyl chloride 1939-99-7, α-Toluenesulfonyl chloride 2386-60-9, 1-Butanesulfonyl chloride 7143-01-3, Methanesulfonic anhydride 13360-57-1, Dimethylsulfamoyl chloride 14077-58-8, Ethoxyacetyl chloride 16629-19-9, 2-Thiophenesulfonyl chloride 39061-97-7, 4-Chloro-3-nitroquinoline 105627-79-0, Isoquinoline-5-sulfonyl chloride hydrochloride 195711-99-0 210303-90-5 210304-10-2 313350-30-0
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RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of imidazoquinolinesulfonamides as inducers of cytokine

biosynthesis)

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642473-94-7P 642473-95-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of imidazoquinolinesulfonamides as inducers of cytokine biosynthesis)

RE.CNT 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD

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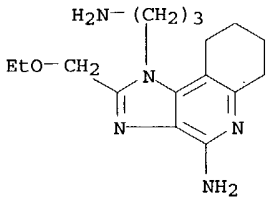
=> s l10 and ethoxymethyl
24478 ETHOXYMETHYL
L11 12 L10 AND ETHOXYMETHYL

=> d scan

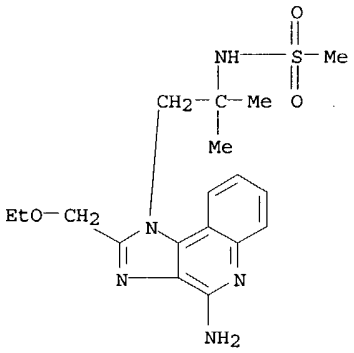
L11 12 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN **1H-Imidazo[4,5-c]quinoline-1-propanamine, 4-amino-2-(ethoxymethyl)-6,7,8,9-tetrahydro- (9CI)**
MF C16 H25 N5 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):11

L11 12 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN **Methanesulfonamide, N-[2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethyl]- (9CI)**
MF C18 H25 N5 O3 S



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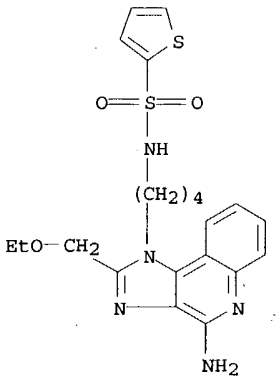
L11 12 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN **2-Thiophenesulfonamide, N-[4-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]butyl]-, mono(trifluoroacetate) (9CI)**
MF C21 H25 N5 O3 S2 . C2 H F3 O2

CM 1



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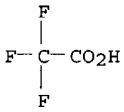
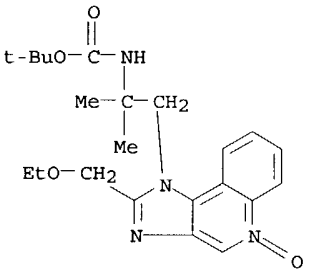


L11 12 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN **Carbamic acid, [2-[2-(ethoxymethyl)-5-oxido-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethyl]-, 1,1-dimethylethyl ester (9CI)**
MF C22 H30 N4 O4



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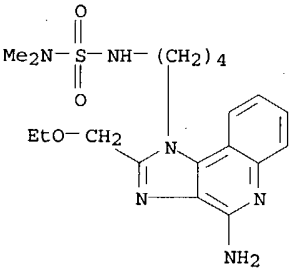
L11 12 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN **Sulfamide, N'-[4-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]butyl]-N,N-dimethyl-, mono(trifluoroacetate) (9CI)**
MF C19 H28 N6 O3 S . C2 H F3 O2

CM 1



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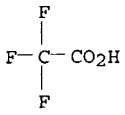
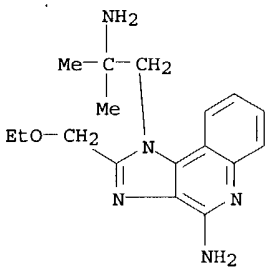


L11 12 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN **1H-Imidazo[4,5-c]quinoline-1-ethanamine, 4-amino-2-(ethoxymethyl)-α,α-dimethyl- (9CI)**
MF C17 H23 N5 O



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IN **Methanesulfonamide, N-[3-[4-amino-2-(ethoxymethyl)-6,7,8,9-tetrahydro-1H-imidazo[4,5-c]quinolin-1-yl]propyl]- (9CI)**
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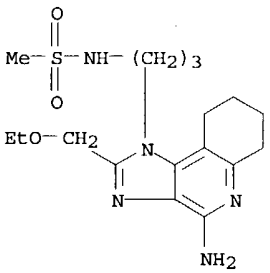

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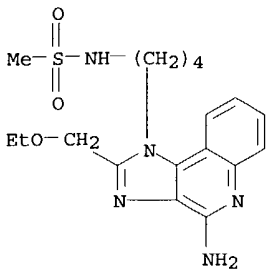
L11 12 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN **Methanesulfonamide, N-[4-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]butyl]-, mono(trifluoroacetate) (9CI)**
MF C18 H25 N5 O3 S . C2 H F3 O2

CM 1



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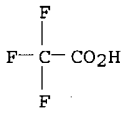
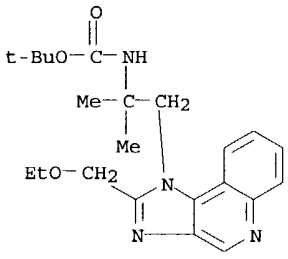


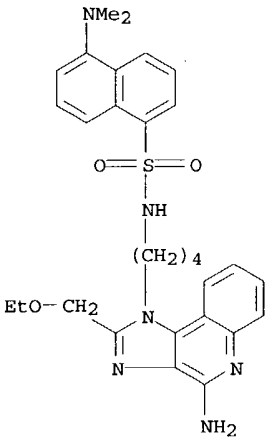
L11 12 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN **Carbamic acid, [2-[2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethyl]-, 1,1-dimethylethyl ester (9CI)**
MF C22 H30 N4 O3



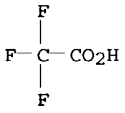
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 12 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN **1-Naphthalenesulfonamide, N-[4-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]butyl]-5-(dimethylamino)-, mono(trifluoroacetate) (9CI)**
MF C29 H34 N6 O3 S . C2 H F3 O2

CM 1



CM 2



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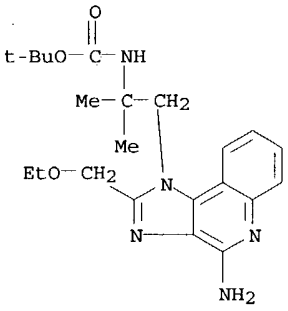
IN **Carbamic acid, [2-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]-1,1-dimethylethyl]-, 1,1-dimethylethyl ester (9CI)**
MF C22 H31 N5 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN **Methanesulfonamide, N-[3-[4-amino-2-(ethoxymethyl)-1H-imidazo[4,5-c]quinolin-1-yl]propyl]- (9CI)**
MF C17 H23 N5 O3 S

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